Fuel 208 (2017) 137–148

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Investigation of ignition characteristics and performance of a neat n-butanol direct injection compression ignition engine at low load

Tadanori Yanai *, Geraint Bryden, Shouvik Dev, Graham T Reader, Ming Zheng

Department of Mechanical, Automotive and Materials Engineering, University of Windsor, 401 Sunset Ave., Windsor, ON N9B 3P4, Canada

HIGHLIGHTS

- Neat n-butanol ignition characteristics in a direct injection CI engine were discussed.
- Chemical kinetic simulations were conducted to analyze the ignition characteristics.
- The combustion and emission characteristics at low load were discussed.

ARTICLE INFO

Article history:
Received 14 January 2017
Received in revised form 17 June 2017
Accepted 20 June 2017

Keywords:
Neat n-butanol
Compression ignition engine
Ignition
Combustion
Emissions
Chemical kinetics simulation

ABSTRACT

Neat (100%) n-butanol was implemented in a direct injection (DI) compression ignition (CI) engine. The ignition, combustion, and emission characteristics at low engine load (below 6.5 bar IMEP), including near idling, were investigated. The engine experiments were performed using a modern common rail type single cylinder DI CI engine with a compression ratio of 18.2:1. Chemical kinetic simulations were also conducted to analyze the ignition characteristics of the experiments. The research results showed that neat n-butanol could not be auto-ignited at normal intake temperature and pressure conditions due to its low reactivity. However, the use of a high intake pressure of 0.75 bar gauge, and an injection timing of −26° ATDC at 5.0 bar IMEP, enabled auto-ignition even without the use of intake heating. One possible reason for this was attributed to the enhancement of the low temperature reaction regime. The ignition timing advancement sensitivity to intake pressure was approximately 1.0 °CA/0.1 bar at 5.0 bar IMEP, and a higher intake pressure allowed a wider injection timing range. A neat n-butanol fueled DI CI engine had a five times longer ignition delay and a 85% longer combustion duration than the same engine fueled with diesel at 2.0 bar IMEP. However, the combustion duration tended to shorten rapidly with increasing engine load, which was the opposite tendency to diesel. At low load, the nitrogen oxides (NOx) and soot emissions were very low compared to those of diesel, whereas the total hydrocarbons (THC), formaldehyde (HCHO), and carbon monoxide (CO) were higher than those of diesel. Carbon dioxide (CO_2) emission was lower than that of diesel. This could be due to the reduced CO oxidation and the lower carbon content in n-butanol. Finally, by combining the previously published results with these results in this research, fuel injection strategies and intake oxygen conditions required to achieve low NOx (≤0.60 g/kWh) and soot (≤0.02 g/kWh) emissions and moderated maximum cylinder pressure rise rate (≤10 bar/°CA) were summarized over a wide load range of 2.0–11.5 bar IMEP.

1. Introduction

The application of fuels derived from biomass to compression ignition (CI) engines is necessary for addressing serious current social issues such as reduction of carbon dioxide (CO_2) emissions, energy security concerns, and air pollution. Several types of biomass fuels for CI engines such as biodiesel [1], biomass to liquid (BTL) using the Fischer–Tropsch process [2,3], dimethyl ether (DME) [4,5], and alcohols [6,7] have been proposed. Among these, alcohols such as ethanol and butanol can be made from biomass sources such as starch (from corn or wheat for instance) and

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Abbreviations: ATDC, after top dead center; BDC, bottom dead center; CA, crank angle [°]; CA5, the crank angle at 5% of mass fraction burned [°ATDC]; CA50, the crank angle at 50% of mass fraction burned [°ATDC]; CA95, the crank angle at 95% of mass fraction burned [°ATDC]; CLD, chemiluminescence detector; CO, carbon monoxide; CO_2, carbon dioxide; COV_{imep}, coefficient of variation of IMEP [%]; DI, direct injection; $dp/d\Theta_{max}$, maximum cylinder pressure rise rate [bar/°CA]; EGR, exhaust gas recirculation; FID, flame ionization detector; FFT, fast Fourier transform; FTIR, Fourier transform infrared spectroscopy; HCHO, formaldehyde; IMEP, indicated mean effective pressure [bar]; LHV, lower heating value [MJ/L]; msec, millisecond; Ne, engine speed [rpm]; NDIR, non-dispersive infrared; NOx, nitrogen oxides; O_2, oxygen; p_{inj}, injection pressure [bar]; p_{max}, maximum cylinder pressure [bar]; PFI, port fuel injection; PMA, paramagnetic analyzer; TDC, top dead center; THC, total hydrocarbons; Φ, equivalence ratio.

* Corresponding author.

E-mail address: tyanai@uwindsor.ca (T. Yanai).

http://dx.doi.org/10.1016/j.fuel.2017.06.096
0016-2361/

cellulose through fermentation [8–10], which is a biological process, unlike BTL. Alcohols are in liquid state under normal temperature, unlike DME, which is gas phase. They have superior oxidation stability and low temperature fluidity compared to biodiesel. Thus, alcohols have better fuel handling characteristics for engine use in comparison to biodiesel and DME.

Among alcohols, n-butanol is a C-4 straight chain alcohol with a molecular formula of C_4H_9OH. Compared to ethanol which is one of the most commonly used bio-alcohols, n-butanol has several advantages. For example, the lower heating value (LHV) of n-butanol (shown in Table 1) is approximately 28% greater by volume, potentially resulting in lower fuel consumption per unit distance. Additionally, a modification to inject larger amounts of fuel such as a large nozzle hole diameter may not be required. The tendency of water absorption is lower, and thus corrosion problems are less severe. This means that n-butanol can potentially be applied to an existing fuel infrastructure, and can be stored in the fuel tank for a longer time. n-Butanol also has better miscibility with diesel, thus a higher percentage of blending is possible. The kinematic viscosity of n-butanol [11] is higher than ethanol, as a result, better wear characteristics between the moving parts of the fuel injection system may be expected. Furthermore, the cetane number of n-butanol [9,12,13] is higher, resulting in easier auto-ignition in CI engines. On the other hand, the drawbacks of using n-butanol are that it can corrode plastic parts and cause swelling of rubber components [9]. However, the latter problem can be overcome by changing the rubber sealing materials to alcohol tolerant products. The production of n-butanol is presently lower than that of ethanol, and the price of n-butanol is also higher than that of ethanol [14,15]. However, in recent years, efficient and economical bio-butanol production techniques have been developed [10,16]. Thus, it is anticipated that as the production of n-butanol increases, the cost will become more competitive. From the above aspects, n-butanol can be expected to become a promising biofuel for CI engines in the future.

Due to the aforementioned benefits, n-butanol has been researched as a fuel for CI engines [17–28]. In 1981, Miller et al. [17] reported the impact of n-butanol blended with diesel fuel on torque output and energy efficiency of a four-cylinder 3.6 liter CI engine. No significant reduction in engine torque was indicated as n-butanol was blended up to 50%. However, an increase in engine knock was observed in the 50% blending case. Thus, up to 30 to 40% blend ratio was suggested to avoid engine knock. Rakopoulos et al. [19] investigated the effect of the n-butanol diesel blend ratio on the performance and emissions of a high speed direct injection (DI) diesel engine. They reported that smoke density was significantly reduced with increasing percentages of n-butanol in the blend. Nitrogen oxides (NOx) were also slightly reduced with the blended fuel. Valentino et al. [20] evaluated the potential of n-butanol diesel blends to improve emissions under premixed low temperature combustion using a turbocharged DI diesel engine. They reported that a 20% and 40% blend by volume of n-butanol and diesel enabled smoke emissions to be drastically reduced. Choi et. al. [21] measured particle matter (PM) size distribution characteristics of diesel engine fuelled with n-butanol diesel blends using a Scanning Mobility Particle Sizer (SMPS). When 20% blending ratio was used, the total PM mass reduced, but nano-size PM (under 50 nm) increased. They also reported that NOx emissions were reduced when the blended fuel was used. Chen et al. [22] studied the impact of n-butanol blend (40% by volume fixed) with diesel on engine performance, and they also conducted simulations to analyze the experimental results. In the 40% blending case, NOx emission increased since a wide high temperature area was formed in the combustion chamber during combustion. The soot emissions were reduced because of a lowered equivalence ratio and better equivalence ratio uniformity, however the total hydrocarbons (THC) and carbon monoxide (CO) emissions increased. The cause of the increase in CO was attributed to a reduced in-cylinder gas temperature during the late expansion process. The indicated thermal efficiency was slightly reduced. Simultaneous reduction of NOx and soot emissions was achieved when approximately 40% exhaust gas recirculation (EGR) was applied. From the literature review above, the main impact on exhaust emissions of a DI CI engine from the blending of n-butanol was a considerable reduction in smoke emissions. Thus, if neat n-butanol is applied to CI engines, even lower smoke may be anticipated, and net CO_2 emissions could be further reduced since a larger amount of renewable fuel is being used in pure form rather than in a blend. It has been reported that neat n-butanol can be applied in spark ignition (SI) engines [29,30]. Hence, if it is possible for n-butanol to be substituted as the main fuel for both SI and CI engines, it could minimize the use of fossil fuels in engines, and the usage of n-butanol would be further promoted. Furthermore, concerns of a phase separation between n-butanol and diesel, and variation of the blending ratio can be ignored when neat n-butanol is used. Therefore, applicability of neat n-butanol as a fuel to DI CI engines needs to be investigated.

Table 1
Fuel properties.

	Diesel Fuel	Ethanol	n-Butanol
Formula	$C_nH_{1.8n}$	C_2H_5OH	n-C_4H_9OH
Density [kg/m^3]	858	780	810
Oxygen Mass [%]	0.0	34.8	21.6
Octane Number	–	108	96
Cetane Number	45.0	2–11 [9,12]	17–25 [9,12,13]
LHV [MJ/kg]	42.1	26.8	33.1
LHV [MJ/L]	36.2	20.9	26.8
Stoic. A/F ratio	14.4	9.0	11.1
Boiling Point [°C]	189.0–345.0	78.4	117.5
$Q_{evaporation}$ [kJ/kg]	316.6	904	582
Kinematic viscosity [mm^2/s]	2.7@40 °C	1.5@20 °C	2.3@40 °C [11] 3.6@20 °C [11]

Due to the differences between n-butanol and diesel fuel, the anticipated challenges when neat n-butanol is applied to DI CI engines are; the compatibility of the modern diesel high pressure fuel injection system, auto-ignition stability, finding fuel injection and air management strategies to obtain low exhaust emissions and high thermal efficiency, and attaining wide load and speed operating ranges. For the challenges, Yanai et al. [23–26] investigated the characteristics of DI CI engine performance fueled with neat n-butanol. Addition of a fuel lubricity improver to the test fuel and installation of fuel coolers enabled a common rail type modern DI diesel engine to run using neat n-butanol [23,24]. The experimental results indicated that stable neat n-butanol auto-ignition was possible with a compression ratio of 18.2:1 when the intake pressure was boosted [23,24]. At mid-load, the ignition delay was much longer than that of diesel due to a lower reactivity. The premixed combustion was dominant, and the combustion was very rapid. Thus, the engine load was limited to mid load due to the high cylinder pressure rise rate. However, not only near-zero soot but also very low NOx emissions were obtained because of a lean and near homogeneous charge, due to the long ignition delay and fast evaporation. The indicated thermal efficiency was similar to that of diesel. Moreover, NOx emissions were further reduced when the injection pressure increased, since the local equivalence ratio was even lower due to the fast fuel spray dispersion prior to ignition [26]. It was also demonstrated that near top dead center split injection was an effective technique to extend